



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:32 AM BST

PDB ID : 6IZ1
Title : Crystal Structure Analysis of a Eukaryotic Membrane Protein
Authors : Wang, X.H.; Zeng, Y.; Gao, F.; Su, M.; Chen, Y.H.
Deposited on : 2018-12-18
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

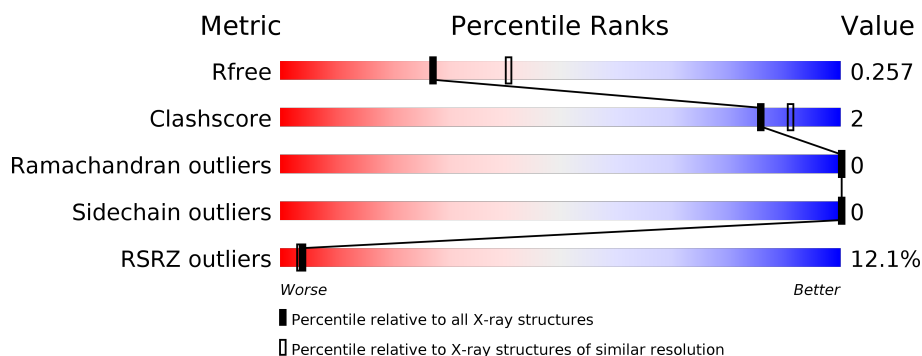
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	<div> <div>8%</div> <div>65%</div> <div>•</div> <div>31%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1896 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Trimeric intracellular cation channel type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	3	0
			1818	1214	290	296	18			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLN	LYS	engineered mutation	UNP Q5ZK43
A	245	SER	CYS	engineered mutation	UNP Q5ZK43
A	297	ALA	-	expression tag	UNP Q5ZK43
A	298	ALA	-	expression tag	UNP Q5ZK43
A	299	ALA	-	expression tag	UNP Q5ZK43
A	300	GLU	-	expression tag	UNP Q5ZK43
A	301	ASN	-	expression tag	UNP Q5ZK43
A	302	LEU	-	expression tag	UNP Q5ZK43
A	303	TYR	-	expression tag	UNP Q5ZK43
A	304	PHE	-	expression tag	UNP Q5ZK43
A	305	GLN	-	expression tag	UNP Q5ZK43
A	306	GLY	-	expression tag	UNP Q5ZK43
A	307	LEU	-	expression tag	UNP Q5ZK43
A	308	GLU	-	expression tag	UNP Q5ZK43
A	309	ASP	-	expression tag	UNP Q5ZK43
A	310	TYR	-	expression tag	UNP Q5ZK43
A	311	LYS	-	expression tag	UNP Q5ZK43
A	312	ASP	-	expression tag	UNP Q5ZK43
A	313	ASP	-	expression tag	UNP Q5ZK43
A	314	ASP	-	expression tag	UNP Q5ZK43
A	315	ASP	-	expression tag	UNP Q5ZK43
A	316	LYS	-	expression tag	UNP Q5ZK43
A	317	HIS	-	expression tag	UNP Q5ZK43
A	318	HIS	-	expression tag	UNP Q5ZK43
A	319	HIS	-	expression tag	UNP Q5ZK43
A	320	HIS	-	expression tag	UNP Q5ZK43
A	321	HIS	-	expression tag	UNP Q5ZK43

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	HIS	-	expression tag	UNP Q5ZK43
A	323	HIS	-	expression tag	UNP Q5ZK43
A	324	HIS	-	expression tag	UNP Q5ZK43
A	325	HIS	-	expression tag	UNP Q5ZK43
A	326	HIS	-	expression tag	UNP Q5ZK43

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Cl	0	0
			5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A:
-
- 8% 65% 31%
- Met Glu Leu Pro Gly Ala Leu Q8 L9 G10 E11 L12 A13 V21 F25 M46 S47 R48 L56 I57 L68 A69 D70 L71 L72 L73 G74 E75 S76 P77 F111 L112 P113 L116 V127 H135 W145 A160 L161 M162 E179 T198 T202 P206 W207
- Lys Glu Glu Lys Asn Glu Gly Thr Arg Lys Arg Lys Ala Glu Glu Ala Glu Glu Asn Leu Leu Thr Phe Phe Glu Glu Leu Glu Asp Tyr Lys Lys Asp Asp Asp Asp Lys His His Thr Ser Ser His His Asn Gln His Gly His Ser His Glu Ala Ser Tyr Gln Pro Pro Pro Val Lys Ser

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.35Å 127.35Å 101.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.49 – 2.40 48.49 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.49-2.40) 91.0 (48.49-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14rc2_3191	Depositor
R, R_{free}	0.217 , 0.257 0.217 , 0.257	Depositor DCC
R_{free} test set	906 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1896	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/1880	0.38	0/2558

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1818	0	1809	8	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	72	0	0	2	0
All	All	1896	0	1809	8	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:HIS:HD2	4:A:555:HOH:O	1.59	0.84
1:A:145:TRP:CZ3	1:A:202:THR:HG22	2.31	0.64
1:A:198:THR:O	1:A:202:THR:HG23	2.03	0.59
1:A:68:LEU:HD11	1:A:162[B]:MET:HG3	1.92	0.52
1:A:46:MET:HE3	4:A:508:HOH:O	2.14	0.46
1:A:127:VAL:HG21	1:A:217:THR:HA	2.00	0.43
1:A:160:ALA:HB1	1:A:179:GLU:HG3	2.00	0.42
1:A:21:VAL:HA	1:A:25:PHE:HB2	2.00	0.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/326 (69%)	224 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/278 (70%)	195 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.



5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/326 (68%)	0.45	27 (12%)  	50, 71, 105, 150	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	LEU	8.0
1	A	10	GLY	6.6
1	A	229	ALA	5.6
1	A	8	GLN	3.4
1	A	73	LEU	3.3
1	A	71	LEU	3.1
1	A	12	LEU	3.0
1	A	48	ARG	2.7
1	A	11	GLU	2.7
1	A	209	GLU	2.7
1	A	111	PHE	2.7
1	A	215	PHE	2.6
1	A	74	GLY	2.6
1	A	206	PRO	2.6
1	A	113	PRO	2.6
1	A	231	HIS	2.6
1	A	72	LEU	2.4
1	A	13	ALA	2.4
1	A	56[A]	LEU	2.4
1	A	116	LEU	2.3
1	A	207	VAL	2.3
1	A	226	PHE	2.2
1	A	69	ALA	2.2
1	A	76	SER	2.2
1	A	112	LEU	2.2
1	A	77	PRO	2.1
1	A	67	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	405	1/1	0.84	0.28	65,65,65,65	1
3	CL	A	404	1/1	0.88	0.13	68,68,68,68	1
3	CL	A	406	1/1	0.94	0.27	57,57,57,57	1
3	CL	A	403	1/1	0.99	0.42	65,65,65,65	1
3	CL	A	402	1/1	0.99	0.23	52,52,52,52	0
2	CA	A	401	1/1	1.00	0.24	49,49,49,49	1

6.5 Other polymers [i](#)

There are no such residues in this entry.